3-Fluoro-6-trifluoromethylbenzamide, N-(3-chlorophenyl)-

Inchi: InChI=1S/C14H8ClF4NO/c15-8-2-1-3-10(6-8)20-13(21)11-7-9(16)4-5-12(11)14(17,18)19

InchiKey: LTZGPILPJHKDQC-UHFFFAOYSA-N

Formula: C14H8ClF4NO

SMILES: O=C(Nc1cccc(Cl)c1)c1cc(F)ccc1C(F)(F)F

Mol. weight [g/mol]: 317.67

Physical Properties

Property code	Value	Unit	Source
gf	-564.93	kJ/mol	Joback Method
hf	-761.68	kJ/mol	Joback Method
hfus	34.73	kJ/mol	Joback Method
hvap	66.30	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.750		Crippen Method
mcvol	191.470	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	2041.00		NIST Webbook
rinpol	2041.00		NIST Webbook
tb	723.34	K	Joback Method
tc	943.81	K	Joback Method
tf	475.23	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.14	J/mol×K	723.34	Joback Method
cpg	507.18	J/mol×K	760.08	Joback Method
cpg	517.28	J/mol×K	796.83	Joback Method
cpg	526.51	J/mol×K	833.57	Joback Method
cpg	534.94	J/mol×K	870.32	Joback Method
cpg	542.65	J/mol×K	907.06	Joback Method
cpg	549.69	J/mol×K	943.81	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358079&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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